

CLAIMS:

1. A method of determining the likelihood of a saccharide composition of a candidate glycan comprising:
  - providing a search mass of a glycan whose composition is to be determined;
  - 5 generating a list of possible glycans made up of components, including monosaccharides, whose total mass is within a predetermined tolerance of the search mass;
  - selecting a reference group of known characterised glycans ;
  - establishing the mean and standard deviation of each component appearing in 10 the reference group of the known characterised glycans ;
  - for each candidate glycan calculating a partial score for each component in that theoretical glycan candidate, the partial score being calculated from the mean and standard deviation of the component appearing in the reference group and which provides a measure of the likelihood of that component being present in the candidate 15 glycan ;
  - combining the partial scores to provide an indication of the likelihood of that candidate glycan occurring.
2. A method as claimed in claim 1 wherein the reference group of glycans 20 comprises glycans of approximately similar mass to the search mass.
3. A method as claimed in claim 1 or 2 wherein the partial scores for each component are based on the difference between the observed number of the component in the candidate glycan composition and the mean for that component in the reference 25 group, divided by the standard deviation and wherein the combining of the partial scores is carried out by multiplying the partial scores together.
4. A method as claimed in claim 1 or 2 wherein the partial score for each component is calculated according to the equation:-

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$$\text{partialscore}_{\text{monosac}} = \frac{\left| \text{mean}_{\text{monosac}} - \text{observed}_{\text{monosac}} \right|}{\text{stdev}_{\text{monosac}}}$$

where  $\text{mean}_{\text{monosac}}$  is the mean number of the given monosaccharide in the reference data set;  $\text{observed}_{\text{monosac}}$  is the number of the given monosaccharide in the

candidate glycan; and  $stddev_{monosac}$  is the standard deviation of the given monosaccharide in the reference data set.

5. A method as claimed in claim 1 or 2 wherein the partial score for each  
5 component is calculated according to the equation:-

$$\text{PartialScore}_m = \frac{e^{-\frac{1}{2}(\text{StDevScore}_m)^2}}{\sqrt{2\pi} \times stddev_m}$$

where  $\text{StDevScore}_m = \text{Abs}(\text{count}_m - \text{mean}_m)/\text{stdev}_m$

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6. A method as claimed in claim 5 wherein the probability of the candidate glycan or "biological index" is calculated according to the equation:

$$\text{biological index} = \frac{1}{\ln\left(\prod_{m \in \text{monosaccharides}} \text{PartialScore}_m\right)}$$

15 7. A method as claimed in any one of claims 1 to 6 wherein the predetermined tolerance of the search mass is within +/- 400Da, preferably +/- 200Da.

8. A system for determining the likelihood of saccharide composition of a candidate glycan comprising a computer means running software implementing the  
20 method of any one of claims 1 to 7.

9. A method of determining the likelihood of a saccharide composition of a candidate glycan using a system as claimed in claim 8 when dependent on any one of claims 2 to 6 including :-

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- inputting a search mass;
- inputting a search mass tolerance;
- inputting a biological index cut off; and
- inputting a maximum value for each component in the candidate composition.